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EXPONENTIAL CONVERGENCE OF ADAPTIVE IMPORTANCE SAMPLING FOR MARKOV CHAINS

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Abstract

We consider adaptive importance sampling for a Markov chain with scoring. It is shown that convergence to the zero-variance importance sampling chain for the mean total score occurs exponentially fast under general conditions. These results extend previous work in Kollman (1993) and in Kollman *et al.* (1999) for finite state spaces.

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1. Introduction

The purpose of this work is to establish conditions for exponential convergence of learning algorithms for Markov chains with scoring. Such chains arise in particle transport and have application to wide-ranging fields, including nuclear reactor operations, well logging for oil exploration, and radiation dosage calculations for exposure to medical X-rays. Computer simulation is an effective approach to such problems (Lux and Koblinger (1991)) and is an alternative to expensive physical experiments.

Simulation of the 'analog' chain (using the transition probabilities for the natural process) is often so time-consuming as to be impractical, for instance, for estimating rare event probabilities. This difficulty is alleviated by importance sampling, wherein rare events are preferentially generated using a different probability mechanism. While importance sampling produces marked improvement, variances still decrease as $\mathcal{O}(1/n)$, where n is the number of simulation runs. There exist zero-variance importance sampling schemes which give exact results in a single run, but with the drawback that the solution must be known in order to construct the zero-variance scheme.

Learning algorithms have been developed to simulate from approximate zero-variance importance functions, and then use the results to improve the importance function. When

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the procedure is iterated, it has been shown numerically (Booth (1985, 1989)) to converge exponentially to the solution. The first theoretical basis for this phenomenon was given by Kollman (1993) and Kollman *et al.* (1999) for finite state spaces. In this work, it is shown that mild constraints (primarily Assumption 3.2 in Section 3) are sufficient to guarantee such convergence for general state spaces.

In Section 2, the problem is formally defined and notation is introduced. In Section 3 we discuss the conditions needed and establish some preliminary results. In Section 4, the theorem on exponential convergence is stated and proved. An idealized particle transport problem is treated by adaptive importance sampling in Section 5, and concluding remarks are found in Section 6.

2. Notations and definitions

2.1. Basic definitions

Consider a Markov chain $\langle X_t : t = 0, 1, 2, \ldots \rangle$ with state space E equipped with a σ-field $\mathcal{E}$ of measurable sets. The transition kernel for the natural process is denoted by $P : E \times \mathcal{E} \longrightarrow [0, 1]$, where $P(x, A) = \mathrm{P}[X_{t+1} \in A \mid X_t = x]$. In keeping with applications of interest, we assume that E is transient, i.e.

$$\sum_{n=0}^{\infty} P^n(x, E) < \infty, \quad \forall x \in E. \tag{1}$$

To account for the remaining probability, we create a *cemetery state* $\Delta \notin E$. The cemetery is absorbing in that $P(\Delta, \Delta) = 1$, and transience means that

$$\mathrm{P}_{x,P}[\tau < \infty] = 1, \quad \forall x \in E, \tag{2}$$

for the transition $\tau = \inf\{t : X_t = \Delta\}$ at which death occurs. The equivalence of (1) and (2) is proved in Revuz (1975).

In particle transport problems, a state has components for particle location, direction, energy, and items related to other aspects of interest (e.g., clock time). Sample paths $\langle X_t \rangle$ are called *particle histories*. Here t denotes the number of collisions and X_t is the state of the particle immediately after the tth collision (e.g. X_t may be the location of the tth collision and momentum of the particle as it departs the collision). Often, the particle makes exponentially distributed steps between collisions with nuclei, at which point it is either scattered or absorbed. The post-scattering direction and energy are determined from the pre-scattering direction and energy and the particular species of nucleus with which the particle collides. The cemetery state Δ corresponds to the particle being absorbed in a collision or else escaping the region of interest, presumed never to return. A simple example of one-dimensional particle transport is discussed in Section 5 below.

Write $\bar{E} = E \cup \{\Delta\}$ and extend P to $\bar{E}$ by defining $P(x, \{\Delta\}) = 1 - P(x, E)$. The overarching probability measure for the chain is denoted by $\mathrm{P}_{x,P}$ where x is an initial state ($X_0 = x$), and $\mathrm{E}_{x,P}$ is the corresponding expectation operator. The set of bounded measurable real valued functions on $\bar{E}$ is denoted by $\mathcal{B}$ and the subset of non-negative elements of $\mathcal{B}$ is denoted by $\mathcal{B}_+$. Whenever we write $h \in \mathcal{B}$, it is assumed that $h(\Delta) = 0$. The transition operator with integral kernel $P(x, \mathrm{d}y)$ is

$$Ph(x) = \int P(x, \mathrm{d}y)h(y), \quad h \in \mathcal{B},$$

and the n-step transition kernel is denoted by P^n.

The objective is to estimate the *expected total score* or *importance function*

$$\mu(x) \equiv \mathrm{E}_{x,P}\left[\sum_{t=1}^{\tau} s(X_{t-1}, X_t)\right] \tag{3}$$

where $s : E \times \bar{E} \longrightarrow [0, \infty)$ is a given *score function*. One example of a score function $s(x, y)$ is the energy loss in going from x to y multiplied by the indicator of a region, so the expected total score is the energy released per particle in the region. The upper limit of the summation in (3) can be extended to ∞ by adopting the convention

$$s(\Delta, x) = 0, \quad \forall x \in \bar{E} \Rightarrow \mu(\Delta) = 0. \tag{4}$$

We usually follow the convention that functions defined on E extend to $\bar{E}$ by $\Delta \mapsto 0$, so $\mu(\Delta) = 0$ conforms with this convention.

2.2. Importance sampling

The simplest way to estimate $\mu(x)$ is to simulate particle histories using the analog kernel P starting at the state x and average the resulting scores. For many problems, this is inefficient, so consider simulating chains having transition kernel $Q(x, A)$, where Q denotes the *importance sampling kernel*.

Assumption 2.1. *For Q to be a valid importance sampling kernel for P,* (i) *E must be transient under Q, and* (ii) *Q must dominate P in that $P(x, \cdot) \ll Q(x, \cdot), \forall x \in \bar{E}$.*

Condition (ii) allows application of Radon–Nikodym theory so that integrals w.r.t. $P(x, \cdot)$ can be expressed as integrals w.r.t. $Q(x, \cdot)$ using the Radon–Nikodym derivative

$$\ell_1(x, y) = \frac{\mathrm{d}P(x, \cdot)}{\mathrm{d}Q(x, \cdot)}(y). \tag{5}$$

A more convenient notation that implicitly defines the Radon–Nikodym derivative is

$$P(x, \mathrm{d}y) = Q(x, \mathrm{d}y)\ell_1(x, y). \tag{6}$$

Letting $\mathrm{Law}_{x,P}(X_1, \ldots, X_n)$ denote the distribution of $X_1, \ldots, X_n$,

$$\mathrm{Law}_{x_0,P}(X_1, \ldots, X_n) \ll \mathrm{Law}_{x_0,Q}(X_1, \ldots, X_n), \quad \forall x_0 \in E, \tag{7}$$

and the Radon–Nikodym derivative is

$$\ell_n(x_0, x_1, \ldots, x_n) = \prod_{t=1}^{n} \ell_1(x_{t-1}, x_t). \tag{8}$$

We write L_n to denote the random variable $\ell_n(X_0, X_1, \ldots, X_n)$ where the initial state X_0 is clear from context. Transience and the strong Markov property imply that $\mathrm{P}_{x,P} \ll \mathrm{P}_{x,Q}$ and the Radon–Nikodym derivative is L_τ.

The total weighted score for the importance sampling chain is

$$Y_Q = \sum_{t \geq 1} s(X_{t-1}, X_t)L_t. \tag{9}$$

We have

$$\begin{aligned}\mu(x) &\equiv \mathrm{E}_{x,P}\left[\sum_{t\geq 1} s(X_{t-1}, X_t)\right] \\ &= \mathrm{E}_{x,Q}\left[\left(\sum_{t\geq 1} s(X_{t-1}, X_t)\right) L_\tau\right] \\ &= \mathrm{E}_{x,Q}[Y_Q]. \end{aligned} \tag{10}$$

The quantity inside the expectation in (10) is the usual importance sampling estimator, though we prefer the estimator (9) because the zero-variance chain for this problem is Markov and, often (Glasserman (1993)), variance is reduced.

Conditioning on the first step of the Markov chain, the importance sampling variance $v_Q(x)$ is

$$\begin{aligned} v_Q(x) &\equiv \mathrm{var}_{x,Q}[Y_Q] \\ &= \mathrm{var}_{x,Q}\mathrm{E}_{x,Q}[Y_Q \mid X_1] + \mathrm{E}_{x,Q}\mathrm{var}_{x,Q}[Y_Q \mid X_1] \\ &= \mathrm{var}_{x,Q}[\ell_1(x, X_1)\{s(x, X_1) + \mu(X_1)\}] + \mathrm{E}_{x,Q}[\ell_1^2(x, X_1) v_Q(X_1)] \\ &= \int_{\bar{E}} Q(x, \mathrm{d}y)\ell_1(x, y)^2[s(x, y) + \mu(y)]^2 - \mu(x)^2 \\ &\qquad + \int_{\bar{E}} Q(x, \mathrm{d}y)\ell_1(x, y)^2 v_Q(y). \end{aligned} \tag{11}$$

This gives an integral equation for v_Q, which in operator form is

$$(I - R)v_Q = f. \tag{12}$$

Here, I is the identity operator, R is an integral operator with kernel

$$R(x, \mathrm{d}y) = Q(x, \mathrm{d}y)\ell_1^2(x, y) = P(x, \mathrm{d}y)\ell_1(x, y), \tag{13}$$

and the right-hand side of (12) is

$$f(x) = \mathrm{E}_{x,Q}[\{\mathrm{E}_{x,Q}[Y_Q \mid X_1] - \mu(x)\}^2]. \tag{14}$$

2.3. Zero-variance importance sampling

Conditioning on the first transition and using the Markov property,

$$\mu(x) = \int_{\bar{E}} P(x, \mathrm{d}y)[s(x, y) + \mu(y)], \tag{15}$$

which gives an integral equation for μ. Consider the importance sampling kernel

$$Q_\mu(x, \mathrm{d}y) = P(x, \mathrm{d}y)\frac{s(x, y) + \mu(y)}{\int_{\bar{E}} P(x, \mathrm{d}z)[s(x, z) + \mu(z)]}, \tag{16}$$

$$= \mu(x)^{-1} P(x, \mathrm{d}y)[s(x, y) + \mu(y)], \tag{17}$$

where (15) is used to simplify the denominator in (16). This chain, known as the *zero-variance chain* returns the score $\mu(X_0)$ with probability 1.

Proposition 2.1. *Let Y_{Q_μ} be as in (9). Then $Y_{Q_\mu} = \mu(X_0)$ on the event $[\tau < \infty]$.*

Proof. This is straightforward by induction on the value of τ.

The zero-variance importance sampling chain exists provided (a) $\mu(x) > 0, \forall x \in E$, so that (17) is well defined; and (b) the zero-variance kernel Q_μ is transient.

2.4. Adaptive importance sampling

Adaptive importance sampling uses simulation data to learn $\mu(x)$. The procedure begins with an initial estimate of $\mu(x)$ and substitutes that estimate into the expression for Q_μ to obtain an *approximate zero-variance* (AZV) *kernel*. From the AZV kernel, simulation data are obtained and used to improve the estimate of $\mu(x)$, which is then used to improve the estimate of Q_μ, and the procedure is iterated.

Let $\nu : E \longrightarrow [0, \infty)$ be an estimate of μ such that $\nu(\Delta) = 0$. Its AZV kernel is

$$Q_\nu(x, \mathrm{d}y) = \begin{cases} P(x, \mathrm{d}y)[s(x, y) + \nu(y)]/\zeta_\nu(x) & \text{if } x \in E, \\ P(x, \mathrm{d}y) & \text{if } x = \Delta, \end{cases} \tag{18}$$

where the normalizing constant is (compare with (16))

$$\zeta_\nu(x) = \int_{\bar{E}} P(x, \mathrm{d}y)[s(x, y) + \nu(y)] = \int_{\bar{E}} P(x, \mathrm{d}y)s(x, y) + P\nu(x). \tag{19}$$

A complication in implementation is that μ depends on the initial state x, so $\mu(x)$ must be estimated $\forall x \in E$. A functional form for μ can however sometimes be obtained from (15); i.e. μ belongs to some family μ_β, where β is a finite-dimensional parameter. Then, β can be estimated from simulation data starting in a finite subset of states in E.

3. Statement of assumptions

3.1. Process assumptions

The following imposes the boundedness of $\mu(x)$ and the transience of the AZV chains, conditions that are satisfied in applications of interest.

Assumption 3.1. *The score function $s(x, y)$ is non-negative and satisfies*

$$\sup_{y \in E, z \in \bar{E}} s(y, z) = M < \infty.$$

Assumption 3.2. *There exists $m > 0$ such that*

$$\inf_{x \in E} \sum_{k=1}^{m} \int_E P^{k-1}(x, \mathrm{d}y) P(y, \Delta) s(y, \Delta) > 0. \tag{20}$$

To see the necessity of a requirement like Assumption 3.2, consider the situation where interest lies only in events intermediate to the particle history and $s(x, \Delta) = 0, \forall x \in E$. Then for any AZV kernel, $Q_\nu(x, \Delta) = 0, \forall x \in E$ and the AZV chain is not transient. Simulation of such chains is of no practical value.

Suppose the natural chain is such that there is a positive probability of death within m steps, where m does not depend on the initial state x, that is

$$\inf_{x \in E} \sum_{k=1}^{m} \int_E P^{k-1}(x, \mathrm{d}y) P(y, \Delta) > 0. \tag{21}$$

Then (20) is achieved by introducing *life insurance*. Define

$$s_\delta(x, y) = \begin{cases} s(x, y) + \delta & \text{if } y = \Delta, \\ s(x, y) & \text{if } y \neq \Delta, \end{cases} \tag{22}$$

where $\delta > 0$ is some known constant, a *death benefit*. Because $\tau < \infty$ a.s., the corresponding expected total score is related to the original importance function by

$$\mu_\delta(x) = \mathrm{E}_{x,P}\left[\sum_{t=1}^{\tau} s_\delta(X_{t-1}, X_t)\right] = \mu(x) + \delta,$$

and estimating μ_δ is equivalent to estimating μ.

Lemma 3.1. *Under Assumptions 3.1 and 3.2,*

$$\inf_{x \in E} \sum_{k=1}^{m} \int_E P^{k-1}(x, \mathrm{d}y) P(y, \Delta) > 0. \tag{23}$$

Proof. From Assumption 3.1, $1 \geq s(y, \Delta)/M$ for all $y \in E$, and so

$$\inf_{x \in E} \sum_{k=1}^{m} \int_E P^{k-1}(x, \mathrm{d}y) P(y, \Delta) \geq \inf_{x \in E} \sum_{k=1}^{m} \int_E P^{k-1}(x, \mathrm{d}y) P(y, \Delta) s(y, \Delta)/M.$$

The right-hand side is simply $M^{-1} > 0$ times (20), and thus is strictly positive.

For a function $h \in \mathcal{B}$, define the supremum norm $\|h\| = \sup_{x \in E} |h(x)|$. For T a linear operator on $\mathcal{B}$, define the norm $\|T\| = \sup\{\|Th\| : h \in \mathcal{B} \text{ and } \|h\| = 1\}$. Of course $\|P\| \leq 1$, but transience of AZV chains requires a stronger bound. The next two results follow from standard arguments about Markov processes.

Lemma 3.2. *With m as in Assumption 3.2,* $\|P^m\| < 1$.

Lemma 3.3. *There exists* $\gamma > 0$ *such that* $\sup_{x \in E} \mathrm{E}_{x,P}[\mathrm{e}^{\gamma \tau}] < \infty$.

For later convenience, define

$$\rho = \|P^m\|^{1/m}. \tag{24}$$

Proposition 3.1. $\|\mu^{-1}\|^{-1} < \infty$ *and* $\|\mu\| < \infty$.

Proof. Using Assumption 3.1 and the previous lemma,

$$\sup_{x \in E} \mu(x) = \sup_{x \in E} \mathrm{E}_{x,P}\left[\sum_{t=1}^{\tau} s(X_{t-1}, X_t)\right] \leq M \sup_{x \in E} \mathrm{E}_{x,P}[\tau] < \sup_{x \in E} \mathrm{E}_{x,P}[\gamma^{-1} \mathrm{e}^{\gamma \tau}] < \infty. \tag{25}$$

That $\mu(x)$ is bounded below away from 0 follows from Assumption 3.2 since

$$\mu(x) \geq \mathrm{E}_{x,P}[I_E(X_{\tau-1}) s(X_{\tau-1}, \Delta) I[\tau \leq m]],$$

where $I[\tau \leq m]$ is the indicator function of $\tau \leq m$. This completes the proof. Note that $\|\mu^{-1}\|^{-1} < \infty$ in this proposition is equivalent to $\inf_{x \in E} \mu(x) > 0$. Thus,

$$\kappa = \|\mu\| \|\mu^{-1}\| \tag{26}$$

is well defined.

We shall assume that a positive lower bound on μ is known.

Assumption 3.3. *There is a known* $\delta > 0$ *such that* $\inf_{x \in E} \mu(x) \geq \delta$.

This assumption is not restrictive—see (22) and the discussion about life insurance.

3.2. Model and estimation method

Next, we assume a parametric linear model for $\mu(x)$. This permits the use of finitely many simulations to estimate $\mu(x)$ for all $x \in E$.

Assumption 3.4. *The function* $\mu(x)$ *is given by*

$$\mu(x) = B_0(x) + \sum_{i=1}^{p} \beta_i B_i(x) = B_0(x) + \boldsymbol{\beta}^T \boldsymbol{B}(x), \tag{27}$$

where $B_0, B_1, \ldots, B_p$ *are known linearly independent basis functions, the* β_i*'s are unknown coefficients,* $\boldsymbol{B}(x)^T = (B_1(x), \ldots, B_p(x))$, *and* $\boldsymbol{\beta}^T = (\beta_1, \ldots, \beta_p)$.

The simulation data are obtained by starting chains from a set of initial states

$$D = \{x_1, x_2, \ldots, x_d\} \subset E,$$

called the *design*. It is required D be such that all model coefficients are estimable. We consider r independent replicates of the simulation starting from each $x_i \in D$. Let $Y_{ij,Q}$, $1 \leq i \leq d$, $1 \leq j \leq r$, denote the total weighted score as in (9) for the jth particle history starting at $X_0 = x_i$, where Q denotes the transition kernel used. Let

$$\bar{Y}_{i,Q} = \frac{1}{r} \sum_{j=1}^{r} Y_{ij,Q} \quad 1 \leq i \leq d,$$

and let $\bar{\boldsymbol{Y}}_Q$ denote the vector of averages $\bar{\boldsymbol{Y}}_Q = (\bar{Y}_{1,Q}, \bar{Y}_{2,Q}, \ldots, \bar{Y}_{d,Q})$.

Let $\mathbb{R}_+$ denote the set of non-negative real numbers. Probabilities and expectations over the larger probability space wherein the simulations take place are written $\mathbb{P}[\cdot]$ and $\mathbb{E}[\cdot]$, respectively.

Assumption 3.5.

(a) *The design* D *and number of replications* r *are constant over all iterations of the algorithm. The estimator* $\hat{\mu}$ *depends on the data*

$$(Y_{ij,Q} : 1 \leq i \leq d, 1 \leq j \leq r)$$

only through $\bar{\boldsymbol{Y}}_Q$, *and we write* $\hat{\mu}(x; \bar{\boldsymbol{Y}}_Q)$ *to denote the estimate evaluated at* x *for data* $\bar{\boldsymbol{Y}}_Q$.

(b) *The estimate satisfies the same bound as in Assumption 3.3:* $\inf_{x\in E} \hat{\mu}(x) \geq \delta$.

(c) *The mapping* $\bar{Y} \mapsto \hat{\mu}(\cdot; \bar{Y})$ *is continuous from* $\mathbb{R}_+^d$ *to* $\mathcal{B}_+$ *when the latter is equipped with the norm* $\|\cdot\|$.

(d) *Let* $v_Q(x) = \mathrm{var}_{x,Q}[Y_Q]$. *Given any* $\epsilon > 0$, *there exists* r_1 *such that* $r \geq r_1$ *implies for all* Q *that*

$$\mathbb{E}[\|\hat{\mu} - \mu\|^2] \leq \epsilon \|v_Q\|. \tag{28}$$

Many approaches to using simulation data for estimation satisfy Assumption 3.5 (Baggerly *et al.* (1998), Sections 6.5.4–6.5.6), some of which allow for considerably simpler simulation of importance sampling chains than others. In Section 5, for example, we use ordinary least squares with truncation at δ (to satisfy (b) above).

4. Main theorem

We begin by explicitly describing the learning algorithm. It is assumed that the starting value $\hat{\mu}^{(0)}$ is given (usually from a simulation of the analog chain or from experience with a similar problem). Iterate the following steps for $n \geq 1$:

1. For each state x_i in the design D, simulate r independent replications of the chain starting at x_i with $Q_{\hat{\mu}^{(n-1)}}$ as the transition kernel.
2. Using the simulated data and estimation method, obtain $\hat{\mu}^{(n)}$ and update n.

The main result can now be stated.

Theorem. *Under the assumptions above, there exist constants* $\theta > 0$ *and* r_0 *such that if the learning algorithm is run with* $r \geq r_0$ *replications of the design* D, *then with probability 1,*

$$e^{\theta n}\|\hat{\mu}^{(n)} - \mu\| \longrightarrow 0 \quad \text{as } n \to \infty.$$

4.1. Technical results on AZV chains

Before proving the main theorem, some preliminary results are needed.

Lemma 4.1. *Let* $\eta > 0$ *be given. Then* $\|\nu - \mu\| < \eta$ *implies* $\forall x \in E$:

(i) $\alpha_1\mu(x) < \nu(x) < \alpha_2\mu(x)$, *where* $\alpha_1 = 1 - \eta\|\mu^{-1}\|$ *and* $\alpha_2 = 1 + \eta\|\mu^{-1}\|$.

(ii) $\tilde{\alpha_1}\mu(x) < \zeta_\nu(x) < \tilde{\alpha_2}\mu(x)$, *where* $\tilde{\alpha_1} = 1 - \eta\kappa\|\mu^{-1}\|$ *and* $\tilde{\alpha_2} = 1 + \eta\kappa\|\mu^{-1}\|$.

(iii) *Define* $R_\nu(x, \mathrm{d}y) = Q_\nu(x, \mathrm{d}y)\ell_1^2(x, y)$. *If*

$$\eta < \frac{1-\rho}{\|\mu^{-1}\|(1+\kappa\rho)}, \tag{29}$$

for ρ *as in Lemma 3.3, then* $(I - R_\nu)^{-1}$ *exists on* $\mathcal{B}$ *and equals* $\sum_{n=1}^{\infty} R_\nu^n$, *and*

$$\|(I - R_\nu)^{-1}\| < \frac{\kappa m(\tilde{\alpha_2}/\alpha_1)^{m-1}}{1 - (\tilde{\alpha_2}/\alpha_1)^m \rho^m} < \infty.$$

Proof. Conclusion (i) is elementary. For (ii), we use the alternative form of ζ_ν,

$$\zeta_\nu = \mu + P(\nu - \mu), \tag{30}$$

which can be derived from (19) and (15). Using (30) together with part (i) gives

$$\zeta_\nu \geq (I - P)\mu + \alpha_1 P\mu = \mu - (1 - \alpha_1)P\mu,$$

with an analogous upper bound, which results in

$$-(1 - \alpha_1)P\mu \leq \zeta_\nu - \mu \leq (\alpha_2 - 1)P\mu$$

and hence $\|\zeta_\nu - \mu\| \leq \eta\|\mu^{-1}\|\mu = \eta\kappa\|\mu^{-1}\|\mu$. Part (ii) follows immediately.

For conclusion (iii), we first define the likelihood ratio

$$\ell_{1,\nu}(x, y) = \frac{P(x, \mathrm{d}y)}{Q_\nu(x, \mathrm{d}y)} = \frac{\zeta_\nu(x)}{s(x, y) + \nu(y)}, \tag{31}$$

where the normalizing constant ζ_ν is given in (19). Let I_h denote the operator of multiplication by $h \in \mathcal{B}$, i.e. $I_h g = hg$, $g \in \mathcal{B}$, and note that $\forall h \in \mathcal{B}_+$,

$$R_\nu h(x) = \int_E P(x, \mathrm{d}y)\ell_{1,\nu}(x, y)h(y) \leq \zeta_\nu(x) \int_E P(x, \mathrm{d}y)\frac{h(y)}{\nu(y)} = (I_{\zeta_\nu} P I_{\nu^{-1}} h)(x).$$

The assumption on η implies $\eta \leq \|\mu^{-1}\|^{-1}$ and hence $\alpha_1 > 0$, so $\nu^{-1} < \alpha_1^{-1}\mu^{-1}$, and applying parts (i) and (ii) gives

$$R_\nu \preceq (\tilde{\alpha_2}/\alpha_1) I_\mu P I_{\mu^{-1}}.$$

where the partial order of linear operators on $\mathcal{B}$ is defined by $T_1 \preceq T_2 \Leftrightarrow T_1 h \leq T_2 h \, \forall h \in \mathcal{B}_+$. Iterating this relationship gives $R_\nu^n \preceq (\tilde{\alpha_2}/\alpha_1)^n I_\mu P^n I_{\mu^{-1}}$. The assumption on η also implies $\tilde{\alpha_2}/\alpha_1 < \rho^{-1}$, i.e. $(\tilde{\alpha_2}/\alpha_1)^m \rho^m < 1$. Thus, $\forall h \in \mathcal{B}_+$,

$$\begin{aligned}
\sum_{n=0}^{\infty} R_\nu^n h &\leq \kappa \sum_{n=0}^{\infty} (\tilde{\alpha_2}/\alpha_1)^n P^n h \\
&= \kappa \sum_{i=0}^{\infty} \sum_{j=1}^{m} (\tilde{\alpha_2}/\alpha_1)^{im+j} P^{im+j} h \\
&\leq \kappa \|h\| \sum_{i=0}^{\infty} (\tilde{\alpha_2}/\alpha_1)^{im} \rho^{im} \sum_{j=1}^{m} (\tilde{\alpha_2}/\alpha_1)^j \|P\|^j \\
&\leq \kappa \|h\| m (\tilde{\alpha_2}/\alpha_1)^m [1 - (\tilde{\alpha_2}/\alpha_1)^m \rho^m]^{-1} \\
&< \infty.
\end{aligned}$$

This shows $(I - R_\nu)^{-1} = \sum_{n=0}^{\infty} R_\nu^n$ exists and gives an upper bound on its norm.

Lemma 4.2. *If $\nu(x) > 0$ for all $x \in E$, $\|\nu\| < \infty$, and $\|\nu^{-1}\| < \infty$, then there exists $\gamma_0 > 0$ such that for all $\gamma < \gamma_0$, $\sup_{x \in E} \mathrm{E}_{x, Q_\nu}[\mathrm{e}^{\gamma\tau}] < \infty$. In particular, the AZV chain is transient on E.*

Proof. Note that for $x \in E$,

$$0 < \zeta_\nu(x) = \int_{\bar{E}} P(x, \mathrm{d}y)s(x, y) + P\nu(x) \leq M + \|\nu\|,$$

where M is given in Assumption 3.1. Hence, the likelihood ratio satisfies

$$\begin{aligned}\ell_{1,\nu}(x, y) &= P(x, \mathrm{d}y)/Q_\nu(x, \mathrm{d}y) = \zeta_\nu(x)/[s(x, y) + \nu(y)] \quad \forall x \in E, \forall y \in \bar{E} \\ &\leq [M + \|\nu\|]/\|\nu^{-1}\|^{-1}.\end{aligned}$$

Define

$$C_\nu = 1/\{\|\nu^{-1}\|[M + \|\nu\|]\}, \tag{32}$$

and note that $C_\nu \leq 1$ since $\|\nu\|\|\nu^{-1}\| \geq 1$. An induction argument shows

$$Q_\nu^k(x, \mathrm{d}y)/P^k(x, \mathrm{d}y) \geq C_\nu^k \quad \forall k > 0, \forall x \in E, \forall y \in \bar{E}.$$

Thus, for all $x \in E$, and m and ρ as in Assumption 3.2 and (24), respectively,

$$\begin{aligned}\mathrm{P}_{x,Q_\nu}[\tau \leq m] &= \sum_{k=1}^{m} \mathrm{P}_{x,Q_\nu}[\tau = k] \\ &= \sum_{k=1}^{m} \int_E Q_\nu^{k-1}(x, \mathrm{d}y)Q_\nu(y, \Delta) \\ &\geq \sum_{k=1}^{m} C_\nu^k \int_E P^{k-1}(x, \mathrm{d}y)P(y, \Delta) \\ &= \sum_{k=1}^{m} C_\nu^k \mathrm{P}_{x,P}[\tau = k] \\ &\geq C_\nu^m \sum_{k=1}^{m} \mathrm{P}_{x,P}[\tau = k] \\ &= C_\nu^m \mathrm{P}_{x,P}[\tau \leq m] \\ &\geq C_\nu^m (1 - \rho^m) \\ &> 0.\end{aligned}$$

This implies that

$$\|Q_\nu^m\| = \sup_{x \in E} Q_\nu^m(x, E) < 1, \tag{33}$$

which gives the desired result (see the comments related to (24) preceding Lemma 3.3).

Lemma 4.3. *If* $\nu \in \mathcal{B}_+$ *and* $\inf_{x \in E} \nu(x) > 0$, *then* $\inf_{x \in E} \zeta_\nu(x) > 0$.

Proof. First, for m as in Assumption 3.2, there must exist $E_0 \subset E$ such that

$$\inf_{x \in E} \sum_{k=1}^{m} \int_{E_0} P^{k-1}(x, \mathrm{d}y)P(y, \Delta)s(y, \Delta) > 0.$$

Note that

$$\begin{aligned}\zeta_\nu(x) &= P(x, \Delta)s(x, \Delta) + \int_E P(x, \mathrm{d}y)[s(x, y) + \nu(y)] \\ &\geq P(x, \Delta)s(x, \Delta) + P(x, E)\|\nu^{-1}\|^{-1} + \int_E P(x, \mathrm{d}y)s(x, y) \\ &\geq P(x, \Delta)s(x, \Delta) + P(x, E)\|\nu^{-1}\|^{-1}. \end{aligned} \tag{34}$$

To prove the lemma by contradiction, suppose $\zeta_\nu(x_k) \to 0$ for some sequence $\langle x_k \rangle$ in E. By taking a subsequence if necessary, either $\langle x_k \rangle$ is in E_0 or in $E - E_0$. If $\langle x_k \rangle$ is in E_0,

$$\begin{aligned}\inf_{x \in E} \mathrm{E}_{x,P}[I_{E_0}(X_{\tau-1})s(X_{\tau-1}, \Delta)I[\tau \leq m]] \\ \leq \mathrm{E}_{x_k,P}[s(X_{\tau-1}, \Delta)I[\tau = 1]] + M\mathrm{P}_{x_k,P}[\tau > 1] \\ = P(x_k, \Delta)s(x_k, \Delta) + MP(x_k, E)\end{aligned}$$

where the latter quantity tends to 0 since both terms in (34) tend to 0 if $\zeta_\nu(x)$ tends to 0. Assuming then that the sequence $\langle x_k \rangle$ is in $E - E_0$, we have

$$\begin{aligned}\inf_{x \in E} \mathrm{P}_{x,P}[\tau < m \cap X_{\tau-1} \in E_0] &\leq \mathrm{P}_{x_k,P}[X_{\tau-1} \in E_0] \\ &\leq \mathrm{P}_{x_k,P}[\tau > 1] \\ &= P(x_k, E),\end{aligned}$$

and the latter tends to 0 if $\zeta_\nu(x_k) \to 0$. Either way we obtain a contradiction to Assumption 3.2, proving the lemma.

Lemma 4.4. *There exist constants K and $\eta > 0$ such that for all $\nu \in \mathcal{B}$,*

$$\|\nu - \mu\| < \eta \Longrightarrow \|\nu_\nu\| < K\|\nu - \mu\|^2.$$

Proof. From (14) we may write f_ν as

$$f_\nu(x) = \mathrm{E}_{x,Q_\nu}[\{\ell_{1,\nu}(x, X_1)[s(x, X_1) + \mu(X_1)] - \mu(x)\}^2], \tag{35}$$

where $\ell_{1,\nu}$ is given in (31). Thus we seek an upper bound on

$$\begin{aligned}\ell_{1,\nu}(x, y)[s(x, y) + \mu(y)] - \mu(x) &= \frac{[\zeta_\nu(x) - \zeta_\mu(x)]s(x, y)}{s(x, y) + \nu(y)} + \frac{\zeta_\nu(x)\mu(y) - \zeta_\mu(x)\nu(y)}{s(x, y) + \nu(y)} \\ &= T_1 + T_2, \quad \text{say.}\end{aligned}$$

We proceed to obtain upper bounds on T_1 and T_2.

If η is chosen such that $\eta < \|\mu^{-1}\|^{-1}$, $\|\nu - \mu\| < \eta$ implies $\nu(x) > 0, \forall x \in E$, and

$$\frac{s(x, y)}{s(x, y) + \nu(y)} \leq 1, \quad \forall x, y \in E.$$

Thus,

$$\|T_1\| \leq \|\zeta_\nu - \zeta_\mu\| = \|P(\nu - \mu)\| \leq \|\nu - \mu\|, \tag{36}$$

where the second equality uses the relation (30) and the third uses $\|P\| \leq 1$.

Turning to T_2, if we require on η that for some $\omega \in (0, 1)$ that $\eta < \omega\|\mu^{-1}\|^{-1}$, then $\|\nu - \mu\| < \eta$ implies $\inf_{x\in E} \nu(x) > (1-\omega)\|\mu^{-1}\|^{-1}$. Since $s(x, y) \geq 0$,

$$\begin{aligned}
&\left|\frac{\zeta_\nu(x)\mu(y) - \zeta_\mu(x)\nu(y)}{s(x, y) + \nu(y)}\right| \\
&\quad \leq (1-\omega)^{-1}\|\mu^{-1}\|\{|[\zeta_\nu(x) - \zeta_\mu(x)]\mu(y)| + |\zeta_\mu(x)[\mu(y) - \nu(y)]|\} \\
&\quad \leq (1-\omega)^{-1}\|\mu^{-1}\|\{\|\zeta_\nu - \zeta_\mu\| \cdot \|\mu\| + \|\zeta_\mu\| \cdot \|\nu - \mu\|\} \\
&\quad \leq (1-\omega)^{-1}\|\mu^{-1}\|\{\|\mu\| \cdot \|\nu - \mu\| + \|\mu\| \cdot \|\nu - \mu\|\}, \qquad (37)
\end{aligned}$$

where the last inequality follows from the facts that $\zeta_\mu = \mu$ and $\|P\| \leq 1$. Thus,

$$\|T_2\| \leq 2(1-\omega)^{-1}\kappa\|\nu - \mu\|.$$

Combining this with (36) and substituting into (35) gives, for $\|\nu - \mu\| < \omega\|\mu^{-1}\|^{-1}$,

$$\|f_\nu\| \leq (1 + 2(1-\omega)^{-1}\kappa)^2\|\nu - \mu\|^2.$$

Because $(I - R_\nu)$ is invertible for ν sufficiently close to μ by Lemma 4.1(iii) and (13), we know that v_ν is the unique solution in $\mathcal{B}$ of $(I - R_\nu)v = f_\nu$, provided

$$\eta \leq \frac{1-\rho}{\|\mu^{-1}\|(1+\kappa\rho)},$$

where ρ is given in (24). For the α_i's as given in Lemma 4.1, we also have

$$\|v_\nu\| \leq \|(I - R_\nu)^{-1}\|\|f_\nu\| \leq \frac{\kappa m(\alpha_2/\alpha_1)^m}{[1-(\alpha_2/\alpha_1)^m\rho^m]}(1 + 2(1-\alpha)^{-1}\kappa)^2\|\nu - \mu\|^2.$$

This proves the result with K given by the factor of $\|\nu - \mu\|^2$ in the last display.

Lemma 4.5. *There exist constants $c \in (0, 1)$, $\eta > 0$, $\phi > 0$, and r_1 such that for all $r \geq r_1$, $\|\hat{\mu}^{(0)} - \mu\| < \eta$ implies*

$$\mathbb{P}\{\|\hat{\mu}^{(m)} - \mu\| \leq c^m\|\hat{\mu}^{(0)} - \mu\|, \forall m \mid \mu^{(0)}\} \geq \phi.$$

Proof. Let η be as in Lemma 4.4. By Assumption 3.5(d), if $\epsilon > 0$, we can take r_1 large enough that for all $r \geq r_1$,

$$\begin{aligned}
&\mathbb{E}[\|\hat{\mu}^{(n+1)} - \mu\|^2 I[\|\hat{\mu}^{(n)} - \mu\| < \eta] \mid \hat{\mu}^{(n)}] \\
&\quad = \mathbb{E}[\|\hat{\mu}^{(n+1)} - \mu\|^2 \mid \hat{\mu}^{(n)}] I[\|\hat{\mu}^{(n)} - \mu\| < \eta] \qquad (38) \\
&\quad \leq \epsilon\|v_{\hat{\mu}^{(n)}}\| I[\|\hat{\mu}^{(n)} - \mu\| < \eta] \qquad (39) \\
&\quad \leq \epsilon K\|\hat{\mu}^{(n)} - \mu\|^2 I[\|\hat{\mu}^{(n)} - \mu\| < \eta] \qquad (40)
\end{aligned}$$

where (38) follows from properties of conditional expectation, (39) follows from (28), and (40) from Lemma 4.4. Note that $b = \epsilon K < 1$ implies

$$\mathbb{E}[\|\hat{\mu}^{(n+1)} - \mu\|^2 I[\|\hat{\mu}^{(n)} - \mu\| < \eta] \mid \hat{\mu}^{(n)}] \leq b\|\hat{\mu}^{(n)} - \mu\|^2 I[\|\hat{\mu}^{(n)} - \mu\| < \eta]. \qquad (41)$$

The remainder of the proof follows exactly as in Lemma 2 of Kollman *et al.* (1999).

4.2. Proof of the main theorem

The proof is very similar to that for finite state spaces in Kollman *et al.* (1999). Details are given here only where extension of that work is needed.

The average of the total weighted scores on the nth iteration at the ith design point (i.e. $\bar{Y}_{i,Q_{\hat{\mu}^{(n-1)}}}$) is denoted by $\bar{Y}_i^{(n+1)}$, $1 \le i \le d$. Note that $\mathbb{E}[\bar{Y}^{(n+1)} \mid \hat{\mu}^{(n)}] = \mu(x_i)$, and by Markov's inequality there exists a constant $k > 0$ such that

$$\mathbb{P}[\bar{Y}_i^{(n+1)} \le k\mu(x_i), 1 \le i \le d \mid \hat{\mu}^{(n)}] > \tfrac{1}{2}, \quad \text{a.s.}$$

Define the region in $\mathbb{R}_+^d$

$$R = \{\boldsymbol{y} \in \mathbb{R}^d : 0 \le y_i \le k\mu(x_i), 1 \le i \le d\}.$$

Since this is a compact subset of $\mathbb{R}_+^d$, we know by Assumption 3.5(c) that

$$H = \sup\{\|\hat{\mu}(\cdot; \bar{\boldsymbol{Y}})\| : \bar{\boldsymbol{Y}} \in R\}$$

is finite. Then

$$\mathbb{P}[\|\hat{\mu}^{(n+1)}\| \le H \mid \hat{\mu}^{(n)}] \ge \tfrac{1}{2}. \tag{42}$$

Define $\mathcal{L}_j(\cdot \mid \nu)$ as the conditional distribution of Y_{Q_ν} when starting at x_j, i.e. $\mathcal{L}_j(A \mid \nu) = \mathrm{P}_{x_j,Q_\nu}[Y_{Q_\nu} \in A]$. We show that the mapping $\nu \mapsto \mathcal{L}_j(\cdot \mid \nu)$ is continuous from the norm topology on $\{\nu \in \mathcal{B}_+ : \nu(x) > 0, \forall x \in E, \text{ and } \|\nu^{-1}\| < \infty\}$ to the space of probability measures on $\mathbb{R}$ endowed with the topology of weak convergence. For this it suffices to show the mapping that $\nu \mapsto \mathrm{E}_{x,Q_\nu}[\exp\{\mathrm{i}uY_{Q_\nu}\}]$ is continuous in ν for each $u \in \mathbb{R}$. Fix ν_0 with $\|\nu_0^{-1}\| < \infty$ and consider another $\nu \in \mathcal{B}_+$ with $\|\nu - \nu_0\| < \epsilon$, where ϵ is determined later. Using Radon–Nikodym derivatives,

$$\begin{aligned}
&|\mathrm{E}_{x,Q_\nu}[\exp\{\mathrm{i}uY_{Q_\nu}\}] - \mathrm{E}_{x,Q_{\nu_0}}[\exp\{\mathrm{i}uY_{Q_{\nu_0}}\}]| \\
&\quad \le \sum_{k=1}^{\infty} \mathrm{E}_{x,Q_{\nu_0}}[|\exp\{\mathrm{i}uY_{Q_\nu}\} - \exp\{\mathrm{i}uY_{Q_{\nu_0}}\}| R_k I[\tau = k]] \\
&\quad\quad + \sum_{k=1}^{\infty} \mathrm{E}_{x,Q_{\nu_0}}[|R_k - 1| I[\tau = k]],
\end{aligned} \tag{43}$$

where

$$R_k = \prod_{t=1}^{k} \frac{\zeta_{\nu_0}(X_{t-1})\{s(X_{t-1}, X_t) + \nu(X_t)\}}{\zeta_\nu(X_{t-1})\{s(X_{t-1}, X_t) + \nu_0(X_t)\}}.$$

Examining the factors that make up R_k,

$$\begin{aligned}
&\left|\frac{\zeta_{\nu_0}(x)\{s(x, y) + \nu(y)\}}{\zeta_\nu(x)\{s(x, y) + \nu_0(y)\}} - 1\right| \\
&\quad = \left|\frac{[\zeta_{\nu_0}(x) - \zeta_\nu(x)][s(x, y) + \nu(y)] + \zeta_\nu(x)[\nu(y) - \nu_0(y)]}{\zeta_\nu(x)[s(x, y) + \nu_0(y)]}\right| \\
&\quad \le \frac{\|\zeta_{\nu_0} - \zeta_\nu\|[M + \|\nu\|] + \|\zeta_\nu\|\|\nu - \nu_0\|}{\|\zeta_\nu^{-1}\|^{-1}\|\nu_0^{-1}\|^{-1}} \\
&\quad \le C_1\|\nu - \nu_0\|
\end{aligned}$$

since $\|\zeta_{\nu_0} - \zeta_\nu\| = \|P(\nu - \nu_0)\| \le \|\nu - \nu_0\|$, where $C_1 = 2[M + 2\|\nu_0\| + 2]\|\nu_0^{-1}\|\|\zeta_{\nu_0}^{-1}\|$, and provided $\|\nu - \nu_0\| < \epsilon$ with $\epsilon < \min\{1, \|\zeta_{\nu_0}^{-1}\|^{-1}/2\}$. That $\inf_{x\in E} \zeta_{\nu_0}(x) > 0$ as in Lemma 4.3 ensures that this is valid.

Using $1 - 1/x \le \log x \le x - 1, \forall x > 0$, for $C_1\|\nu - \nu_0\| < \frac{1}{2}$,

$$|R_k - 1| \le \max\{e^{kC_1\|\nu-\nu_0\|} - 1, 1 - e^{-2kC_1\|\nu-\nu_0\|}\} \le e^{kC_1\|\nu-\nu_0\|} - e^{-2kC_1\|\nu-\nu_0\|}.$$

Thus, for the second summation in (43),

$$E_{x,Q_{\nu_0}}[|R_\tau - 1|] \le E_{x,Q_{\nu_0}}[e^{\tau C_1\|\nu-\nu_0\|}] - E_{x,Q_{\nu_0}}[e^{-2\tau C_1\|\nu-\nu_0\|}].$$

Since τ has a moment generating function under $P_{x,Q_{\nu_0}}$ finite in a neighborhood of the origin (Lemma 4.2), the second summation in (43) tends to 0 as $\|\nu - \nu_0\| \to 0$.

Turning to the first summation in (43), arguments similar to the above show that

$$|Y_{Q_\nu} - Y_{Q_{\nu_0}}| \le C_2 M\tau\|\nu - \nu_0\|,$$

for some constant C_2 which depends only on ν_0 and not ν, and provided $\|\nu - \nu_0\| < \epsilon$ for ϵ sufficiently small. Since the derivative of $y \mapsto e^{iuy}$ is uniformly bounded, using previous bounds on R_k,

$$E_{x,Q_{\nu_0}}[|\exp\{iuY_{Q_\nu}\} - \exp\{iuY_{Q_{\nu_0}}\}|R_\tau] \le C_3 E_{x,Q_{\nu_0}}[\tau \exp[C_1\tau\|\nu - \nu_0\|]].$$

Using this and the existence of a moment generating function for τ, the first summation in (43) tends to 0 as $\|\nu - \nu_0\| \to 0$, establishing the continuity.

It now follows by an application of Dini's theorem as in Section 3 of Kollman *et al.* (1999) (see Equation (17) of that paper) that the family of random variables Y_{Q_ν} starting at x_j with probability distributions

$$\{\mathcal{L}_j(\cdot \mid \nu) : \delta \le \nu(x) \le H, \forall x \in E\}$$

is uniformly integrable, that is

$$\lim_{\alpha\uparrow\infty} \sup \left\{ \int_{y>\alpha} y\mathcal{L}_j(dy \mid \nu) : \delta \le \nu(x) \le H, \forall x \in E \text{ and } 1 \le j \le d \right\} = 0.$$

This implies (Parzen (1954)) that the weak law of large numbers holds uniformly over $\{\nu \in \mathcal{B}_+ : \delta \le \nu(x) \le H, \forall x \in E\}$. Thus, for any $\epsilon > 0$, there exists r_2 such that for all $r \ge r_2$,

$$\mathbb{P}[|\bar{Y}_j^{(n+1)} - \mu(x_j)| < \epsilon \mid \hat{\mu}^{(n)}] \ge \tfrac{1}{2}, \tag{44}$$

almost surely on the event $[\delta \le \hat{\mu}^{(n)}(x) \le H, \forall x \in E]$. In view of Assumption 3.5(c), given any $\eta > 0$, we may take ϵ sufficiently small that

$$\mathbb{P}[\|\hat{\mu}^{(n+1)} - \mu\| < \eta \mid \hat{\mu}^{(n)}] \ge \tfrac{1}{2}, \tag{45}$$

almost surely on the event $[\delta \le \hat{\mu}^{(n)}(x) \le H, \forall x \in E]$.

With c, η, ϕ, and r_1 as in Lemma 4.5, let $r_0 = \max\{r_1, r_2\}$. Suppose $r \geq r_0$. The sequence $\langle \hat{\mu}^{(n)} \rangle_{n=0}^{\infty}$ is Markov, so part (b) of Assumption 3.5, (42), and (44) imply

$$\begin{aligned}\mathbb{P}[\|\hat{\mu}^{(n+2)} - \mu\| < \eta \mid \hat{\mu}^{(n)}] &\geq \mathbb{P}[\|\hat{\mu}^{(n+2)} - \mu\| < \eta \mid \delta \leq \hat{\mu}^{(n+1)}(x) \leq H, \forall x \in E] \\ &\quad \times \mathbb{P}[\delta \leq \hat{\mu}^{(n+1)}(x) \leq H, \forall x \in E \mid \hat{\mu}^{(n)}] \\ &\geq \tfrac{1}{4}.\end{aligned}$$

Thus, independently of the value $\hat{\mu}^{(n)}$, if the algorithm is run with $r \geq r_0$ we have at least $\frac{1}{4}$ probability of being within an η-neighborhood of μ in two steps. Letting

$$\lambda_n = \mathbb{P}[\|\hat{\mu}^{(n+2)} - \mu\| < \eta \mid \hat{\mu}^{(n)}],$$

then $\sum_n \lambda_n$ diverges, and by the conditional Borel–Cantelli lemma (Breiman, 1968),

$$\mathbb{P}[\|\hat{\mu}^{(n)} - \mu\| < \eta \text{ i.o.}] = 1. \tag{46}$$

The remainder of the proof in Section 3 of Kollman *et al.* (1999) beginning with Equation (20) goes through verbatim as the nature of the state space plays no role.

5. An example

We consider the 'rod problem,' an idealized particle transport in one dimension. A particle moves along the real line. The interval $[0, T]$ denotes a 'rod' of length T. From an initial location $v \in [0, T]$, the particle moves to the right ($u = +1$) or left ($u = -1$). It travels a distance that is exponentially distributed with mean free path σ^{-1}. Should this path length take the particle outside the rod, the process terminates at the next step. If the path length is too short for escape, the particle collides with an atom. Upon collision, the particle is absorbed with probability $\pi \in (0, 1)$. If the particle is not absorbed, it scatters isotropically (i.e., with equal probability of moving left or right) and again travels a distance that is exponentially distributed with mean σ^{-1}. If it has not escaped the rod, it again collides with an atom. The process continues until the particle either is absorbed or escapes.

A possible state of the particle is denoted by $x = (v, u)$ where

$$v = \text{ particle location } (-\infty < v < \infty), \text{ and } u = \text{ particle direction } (u = \pm 1).$$

The Markov chain is written $X_t = (V_t, U_t)$. (Note that one can construct a Markov chain with only V_t but that efficient importance sampling in many cases will generally give preferential weight to the different values of U_t. For instance, if we want to calculate the probability of exit to the right, which is typical in shielding problems, then we should consider giving more weight to $U_t = +1$.) Initially, v is the location from which the particle is 'sourced' at time 0, and afterwards is the location of the last collision if $0 \leq v \leq T$. The component u is the direction of the particle after its last collision, if it is not absorbed. If the particle is absorbed, it goes directly to Δ. If the particle escapes at step t, i.e. $V_t > T$ or $V_t < 0$, then the particle goes to Δ at step $t + 1$.

Simulation work on this problem has appeared elsewhere (Booth (1997)).

The goal is to estimate the analog probability $\mu_0(x)$ that the particle escapes to the right, corresponding to the score function

$$s_\delta((v, u), y) = \begin{cases} \delta & \text{if } v \leq T \text{ and } y = \Delta, \\ 1 + \delta & \text{if } v > T \text{ and } y = \Delta, \\ 0 & \text{otherwise.} \end{cases} \tag{47}$$

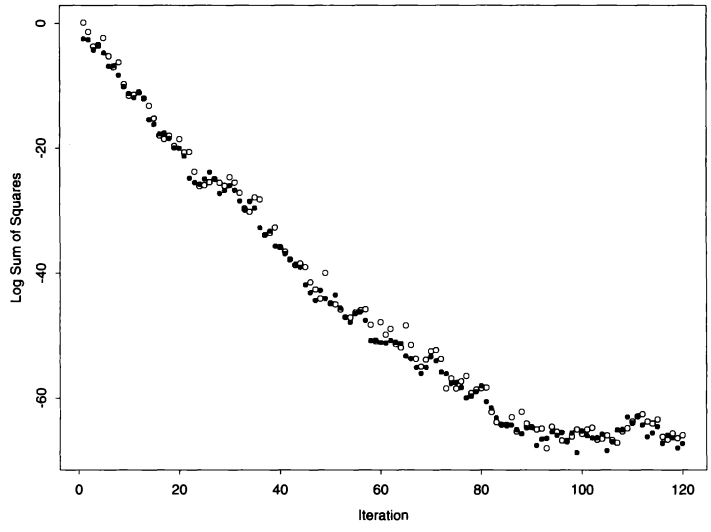

FIGURE 1: Exponential convergence for the rod problem.

The expected score for a particle history is $\mu_\delta(x) = \delta + \mu_0(x)$. A first-principles derivation (Baggerly *et al.* (1998) Section 6.1) shows that

$$\mu_\delta(v, u) = B_0(v, u) + \sum_{j=1}^{4} \beta_j B_j(u, v),$$

where $B_0(v, u) = \delta$ for $v \leq T$, $B_0(v, u) = 1 + \delta$ otherwise, and

$$B_j(v, u) = \begin{cases} \exp[-\sigma v \pi^{1/2}] & \text{if } 0 \leq v \leq T \text{ and either } j = 1 \text{ and } u = +1, \\ & \quad \text{or } j = 3 \text{ and } u = -1; \\ \exp[+\sigma v \pi^{1/2}] & \text{if } 0 \leq v \leq T \text{ and either } j = 2 \text{ and } u = +1, \\ & \quad \text{or } j = 4 \text{ and } u = -1; \\ 0 & \text{otherwise.} \end{cases}$$

We chose mean free path $\sigma^{-1} = 1$, rod length $T = 20$, absorption probability $\pi = 0.1$ per collision, and death benefit $\delta = 0.01$ for the results presented here. We used the design D where a particle is sourced inward from each end of the rod, $(v_i, u_i) = (0, +1)$ and $(20, -1)$, and 18 additional particles were sourced at intermediate states $(v_i, u_i) = (2, \pm 1), (4, \pm 1), \ldots,$ and $(18, \pm 1)$. In each iteration of the algorithm, one replication was used ($r = 1$), and the initial estimate $\hat{\mu}_\delta^{(0)}$ was obtained by simulating the analog chain. To estimate the model parameters β_j, $1 \leq j \leq 4$, we subtracted δ from the observed total weighted scores to account for the term $B_0(v, u)$, used least squares regression to fit the four-parameter model, truncated at zero any negative fitted values, and added δ to the result to obtain $\hat{\mu}_\delta(x)$. The importance sampling kernel was updated accordingly. It can be shown that Assumption 3.5 is satisfied by this approach.

Figure 1 displays the results, where convergence to machine accuracy is achieved in roughly 90 iterations of 20 particle histories each. By comparison, estimating the rare event probability

$\mu_0(0, +1)$, which is roughly 0.001, with a 1% relative error using analog simulation would require $n \approx 10\,000\,000$ particle histories.

Plotted in Figure 1 using solid circles is the log sum of squares $\sum_i (\hat{\mu}(x_i) - \mu(x_i))^2$, where the sum is over the 20 design points. The linear decrease displays the exponential convergence of $\hat{\mu}^{(n)}$ to μ. Also plotted, using open circles, is the log residual sum of squares $\sum_i (Y_{i,Q} - \hat{\mu}(x_i))^2$, which is used in practice to assess convergence.

6. Concluding remarks

We conclude with remarks relevant to practical application. The main theorem provides no guidance for determining the number of replications r. In our experience, insufficient replication is reflected by no improvement in the residual sum of squares during early iterations of the algorithm. This can be overcome (conceptually if not computationally) by increasing r until observing linear decrease such as in Figure 1.

For many problems, a known parametric model for the importance function μ may not exist (the lack of analytical solutions being one reason why computer simulation is widely used). One may approximate μ with a truncated series expansion. With such approximation, a zero-variance solution is not possible, although we see in numerical experiments exponential convergence to a limiting accuracy, after which no further improvement occurs, for example, Example 4 of Kollman *et al.* (1999). From that point on, variance reduction of n^{-1} can be obtained by averaging the observed $\{\hat{\mu}^{(n)}\}$.

Adaptive learning algorithms offer great potential to escape the n^{-1} rate of convergence of variance common to ordinary simulation. The underlying approach is straightforward and simple to implement.

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